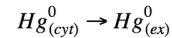
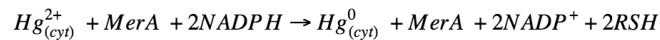
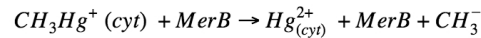
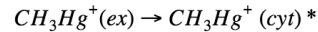


Mathematical Modeling

The reactions below shows the four-step reaction network for the conversion of methylmercury to volatile mercury using the mer operon in *E. coli*. This network involves the transport of methylmercury into the cell, its subsequent conversion into ionic and volatile mercury, and the transport of volatile mercury to the extracellular space. This simplified network follows the proposed mechanism of the mer operon and it captures the primary steps of methylmercury breakdown in *E. coli*.



*According to research done by Mason et al., methylmercury diffuses into the cytosol.

Furthermore, a system of ordinary differential equations was used to model the biochemical reactions taken place at each step of the conversion process. The cofactors were not included in the equations because at sufficient concentrations, they do not significantly alter the rates.

$$\frac{dCH_3Hg^+(cyt)}{dt} = k_1 * [CH_3Hg^+(ex)]$$

$$\frac{dHg^0(ex)}{dt} = k_5 * [Hg^0(cyt)]$$

$$\frac{dHg^{2+}(cyt)}{dt} = \frac{V_b * [CH_3Hg^+(cyt)]}{K_2 + [CH_3Hg^+(cyt)]}$$

$$k_1 = 100000 \text{ nM/hour}$$

$$V_b = 1830000 \text{ nM/hour} \quad K_2 = 1000 \text{ nM}$$

$$V_a = 384000 \text{ nM/hour} \quad K_3 = 12600 \text{ nM} \quad K_4 = 97600 \text{ nM}$$

$$k_5 = 130992 \text{ nM/hour}$$

$$\frac{dHg^0(cyt)}{dt} = \frac{V_a * [Hg^{2+}]_{cyt}}{K_3 + [Hg^{2+}]_{cyt} + [Hg^{2+}]_{cyt}^2 / K_4}$$

The equations used in conversion steps 3 and 4 are extracted from studies done by Maria on ionic mercury uptake by *E. coli* cells (Maria, 2010). These equations can be used because ionic mercury is converted into elemental mercury which in turn diffuses into the extracellular space; these two steps were described in the Maria paper. It is assumed that methylmercury and ionic mercury have similar orders of magnitude of transport rate into the cell.